

AMENDMENTS TO THE CLAIMS

Claims 1 and 2 (CANCELED)

3. (CURRENTLY AMENDED) A computer-implemented method of selecting a set of marker molecules for structural comparisons in a model for molecular behavior prediction~~constructing a model for predicting molecular behavior using marker molecules~~, said method comprising:

receiving data related to one or more chemical or biological properties of a set of structurally defined reference molecules;

using said data, classifying the respective molecules in said a set of reference molecules as either possessing or not possessing at least one property;

selecting a subset of said set of reference molecules, wherein all of the molecules in said subset possess the at least one property;

comparing all molecules in said set with all other molecules in said set in accordance with a pre-defined numerical similarity metric;

selecting a first molecule of said subset;

sorting all other molecules of said set in descending order of numerical similarity to said first molecule, thereby defining a similarity distance in terms of number of molecules between said first molecule and each other molecule of the set;

defining, for each range in molecules of similarity distance away from said first molecule, a fractions-correctly-predicted metric as the number of molecules in said range which are also members of said subset divided by the total number of molecules in said range;

counting the number of molecules away from said first molecule at which the fractions-correctly-predicted metric for said first molecule drops below a threshold value;

choosing ~~selecting a plurality of~~ said first molecule as a marker molecules from the subset, said plurality of marker molecules being less in number than the number of molecules in said subset, if said first molecule has a fractions-correctly-predicted metric which exceeds said threshold value for a pre-selected minimum distance.

4. (ORIGINAL) The method of Claim 3, wherein said subset comprises all of the molecules in said set that possess said at least one property.

Claim 5 (CANCELED)

6. (CURRENTLY AMENDED) The method of Claim 53, additionally comprising repeating said counting step for a plurality of different threshold values.

7. (CURRENTLY AMENDED) The method of Claim 63, comprising repeating said selecting a first molecule, sorting, defining, counting, and choosing steps for other molecules of said subset at a plurality of different threshold values and minimum distances so as to select a plurality of preliminary sets of marker molecules.

8. (ORIGINAL) The method of Claim 7, comprising choosing a final set of marker molecules by making molecular behavior predictions for all molecules in said set using each one of said preliminary sets of marker molecules, and choosing as said final set of marker molecules the preliminary set that most accurately predicts molecular behavior of molecules of said set.

Claims 9-18 (CANCELED)